

# Edge singularities in high-energy spectra of gapped one-dimensional magnets in strong magnetic fields

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We use the dynamical density matrix renormalization group technique to show that the high-energy part of the spectrum of a  $S = 1$  Heisenberg chain, placed in a strong external magnetic field  $H$  exceeding the Haldane gap  $\Delta$ , contains edge singularities, similar to those known to exist in the low-energy spectral response. It is demonstrated that in the frequency range  $\omega \gtrsim \Delta$  the longitudinal (with respect to the applied field) dynamical structure factor is dominated by the power-law singularity  $S^{\parallel}(q = \pi, \omega) \propto (\omega - \omega_0)^{-\alpha'}$ . We study the behavior of the high-energy edge exponent  $\alpha'$  and the edge  $\omega_0$  as functions of the magnetic field. The existence of edge singularities at high energies is directly related to the Tomonaga-Luttinger liquid character of the ground state at  $H > \Delta$  and is expected to be a general feature of one-dimensional gapped spin systems in high magnetic fields.

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## I. INTRODUCTION

Studying spectral response is a valuable tool to reveal the properties of the strongly correlated ground state in interacting electronic systems. One of the paradigmatic concepts in physics of one-dimensional (1d) systems is the so-called Tomonaga-Luttinger liquid (TLL),<sup>1</sup> which for 1d systems plays a similar role as the Fermi liquid theory for higher dimensions. One of the prominent features of the TLL is the absence of a quasiparticle peak in the spectral function; instead, there is a power-law singularity, with a non-universal exponent that depends on the interaction strength.<sup>2,3</sup>

Apart from 1d conductors (e.g., such as carbon nanotubes<sup>4,5</sup>) and edge states in fractional quantum Hall systems,<sup>6,7</sup> the TLL ground state is expected to exist in several other 1d systems, particularly in spin chains and ladders. For an antiferromagnetic (AF)  $S = \frac{1}{2}$  Heisenberg chain, the TLL character of the ground state can be rigorously established from the Bethe ansatz solution,<sup>8</sup> and it is believed<sup>9,10</sup> that this picture is valid also for the other gapless AF chains with half-odd-integer  $S$ .

For AF Heisenberg chains with integer  $S$  and for spin ladders, which have a finite excitation gap  $\Delta$ , it has been argued by analytical<sup>11,12</sup> and numerical<sup>13,14</sup> methods that in an external magnetic field  $H > \Delta$ , strong enough to close the spin gap and cause a finite magnetization, the ground state is also of the TLL type.

Recently, in a search for Luttinger liquid signatures in spin systems, several experimental studies have been undertaken.<sup>15,16,17,18,19</sup> Most of the experimental evidence is, however, indirect, based, e.g., on the analysis of the temperature dependence of specific heat<sup>17,19</sup> or NMR relaxation rate.<sup>18</sup> Direct detection of the low-energy excitation continuum in inelastic neutron scattering experiments<sup>15,16</sup> is a difficult task, not to mention

extracting the dynamical exponents from the low-energy spectrum. High-energy modes might be easier to study, especially with techniques such as electron spin resonance (ESR).<sup>20,21</sup>

At the same time, the high-energy excitations can be viewed as mobile impurities interacting strongly with the underlying TL liquid, and their spectrum can bear similar features as those found in TLL, namely the absence of the quasiparticle peak which is replaced by an edge singularity.<sup>22,23,24,25</sup> It was shown<sup>23</sup> that the spectrum of high-energy excitations with  $S^z = 0, 1$  contains an edge singularity with a nontrivial field dependence of the edge frequency which in the idealized model with no interaction except the hardcore constraint is given by  $\omega_0 = (1 - S^z)H$ . The spectral function of a mobile impurity in the TL liquid has been extensively studied theoretically;<sup>26,27</sup> however, to our knowledge, no numerical results are available to compare with the theoretical predictions. An alternative bosonization description including high-energy modes has been proposed recently.<sup>28</sup> All of this motivates further study of the high-energy spectra of 1d gapped spin systems in strong field.

In the present paper, we study the  $S = 1$  Heisenberg chain, which is a paradigmatic example of a 1d gapped antiferromagnet. There is a large body of numerical and theoretical results concerning its low-energy behavior in strong fields<sup>12,13,14,29</sup> which can be used for consistency checks. Using the dynamical density matrix renormalization group (DMRG) technique, we will show that the high-energy part of the spectrum of a  $S = 1$  chain, placed in a strong external magnetic field  $H$  exceeding the Haldane gap  $\Delta$ , contains edge singularities, similar to the well-known infrared singularities in the low-energy spectral response. It will be demonstrated that in the frequency range  $\omega \gtrsim \Delta$  the longitudinal dynamical structure factor is dominated by the continuum with a power-law edge singularity  $S^{\parallel}(q = \pi, \omega) \propto (\omega - \omega_0)^{-\alpha'}$ .

The edge exponent  $\alpha'$  is found to decrease as a function of magnetization, and the edge  $\omega_0$  is shown to follow approximately the linear law  $\omega_0 \simeq H$  as found earlier.<sup>22,23,24</sup>

## II. THEORETICAL PRELIMINARIES

Consider the  $S = 1$  Heisenberg chain in an applied field described by the Hamiltonian

$$\hat{\mathcal{H}} = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} - H \sum_n S_n^z, \quad (1)$$

where  $\mathbf{S}_n$  is the spin-1 operator at site  $n$ , the exchange constant  $J$  will be set to unity, and the external magnetic field  $H$  is applied along the  $z$  axis. In absence of the applied field, the ground state of the model is a singlet, and the lowest excitations are the triplet of Haldane magnons separated from the ground state by the gap  $\Delta \simeq 0.41$  at the wave vector  $q = \pi$ . The gap closes for  $H > H_c = \Delta$ , and the system acquires a finite density of  $S^z = +1$  magnons, which can be viewed as bosonic particles satisfying the hardcore constraint. It is convenient to redefine the momentum so that the minimum of the magnon dispersion will correspond to zero. Interacting  $S^z = 1$  magnons form a TL liquid with the Hamiltonian given by

$$\mathcal{H}_0 = \frac{v_F}{2} \int dx \left\{ \frac{1}{K} (\partial_x \varphi)^2 + K (\partial_x \theta)^2 \right\}, \quad (2)$$

where  $\varphi$  and  $\theta$  is a pair of bosonic fields satisfying the commutation relations  $[\varphi(x), \theta(x')] = i\Theta(x' - x)$  (here  $\Theta(x)$  is the Heaviside function) and connected by the duality relation  $\partial_t \varphi = v_F \partial_x \theta$ . The physical properties of the TL liquid are completely characterized by its Fermi velocity  $v_F$  and the TLL parameter  $K$ . Both  $v_F$  and  $K$  are functions of  $H$ , and their behavior for the Haldane chain has been studied analytically<sup>12,29</sup> as well as numerically.<sup>13,14</sup> An important feature of the effective TLL description of the Haldane chain is the fact that the parameter  $K$  is always larger than unity ( $K \rightarrow 1$  as  $H \rightarrow H_c$ ).

The local spin density  $\rho(x)$  (i.e., the density of the sea particles) can be expressed as

$$\rho = S^z = m + \frac{1}{\sqrt{\pi}} \partial_x \varphi + \text{const} \times \sin \{2k_F x + \sqrt{4\pi} \varphi\}, \quad (3)$$

where  $m = m(H) \equiv k_F/\pi$  is the equilibrium magnetization density at the given field. The operator  $a^\dagger \sim e^{i\sqrt{\pi}\theta}$  creates a kink in the  $\varphi$  field shifting it by  $\sqrt{\pi}$  and thus corresponds to the creation of a  $S^z = 1$  particle, so that at low energies one can establish the correspondence  $S^+ \sim a^\dagger$ . The low-energy contribution to the transversal dynamical structure factor (DSF) is thus given by  $S^{+-}(q = \pi, \omega) \propto \int dx \int dt e^{i\omega t} \langle a^\dagger(x, t) a(0, 0) \rangle$ , and, since

$$\langle a^\dagger(x, t) a(0, 0) \rangle \propto (v_F^2 t^2 - x^2)^{-\eta/2} \quad \text{with} \quad \eta = \frac{1}{2K},$$

one readily obtains the infrared singularity

$$S^{+-}(q = \pi, \omega) \propto \frac{1}{\omega^\alpha}, \quad \alpha = 2 - \eta \quad (4)$$

with the edge exponent  $\alpha$  determined solely by the TL liquid parameter  $K$ .

To describe the excitation of “impurity” particles corresponding to the higher-energy magnon branch with  $S^z = 0$ , one can introduce another bosonic field  $b(x)$  described by the Hamiltonian

$$\mathcal{H}_b = \int dx \left\{ \omega_0 b^\dagger b + \frac{1}{2M} (\partial_x b^\dagger)(\partial_x b) \right\}. \quad (5)$$

The scaling dimension of the field  $b$  is  $\dim[b] = \frac{1}{2}$ . The TLL action is Lorentz-invariant and thus dictates the dynamical exponent  $z = 1$ , from which one can see that the scaling dimension of the mass  $M$  is equal to  $+1$ , i.e.,  $M$  flows to infinity so that one can neglect the “impurity” dispersion described by the second term in (5); this argument is essentially identical to the dynamical localization of a hole moving in an antiferromagnet as discussed in Ref. 30.

We will be interested in the contribution of the excited “impurity” particles ( $b$ -particles) to the dynamical structure factor  $S^{zz}(q = \pi, \omega)$ , which will be determined by  $b$ -particles with zero momentum. The local interaction between the “impurity” particles and the sea particles ( $a$ -particles) is proportional to the product of corresponding densities  $b^\dagger b \rho$ .<sup>31</sup> This yields, apart from renormalizing the energy  $\omega_0 \mapsto \omega_0 + \text{const} \cdot m$ , two interaction terms: one corresponds to forward scattering and is given by

$$\mathcal{H}_{int}^f = U_f \int dx \frac{1}{\sqrt{\pi}} (\partial_x \varphi) b^\dagger b, \quad (6)$$

and the other, which is proportional to  $b^\dagger b \sin \{2k_F x + \sqrt{4\pi} \varphi\}$ , describes backscattering. The backscattering term, however, is irrelevant since its scaling dimension is  $1 + K$ , and for the Haldane chain one always has  $K > 1$ . With the remaining interaction (6), the Hamiltonian can be diagonalized by means of a unitary transformation<sup>32</sup>

$$\hat{U} = e^{-i\delta \int dx \theta(x) b^\dagger(x) b(x)}, \quad \text{with} \quad \delta = \frac{K U_f}{v_F \sqrt{\pi}}, \quad (7)$$

which changes the phase of  $b$  operator according to

$$b \mapsto \bar{b} = \hat{U}^\dagger b \hat{U} = b e^{-i\delta\theta}. \quad (8)$$

Apart from removing the interaction (6), the unitary transformation (7) just renormalizes the threshold energy  $\omega_0$ , which thus can in principle depend both on the interaction and on the applied field.

Exciting a  $b$ -particle requires “disturbing” the sea of  $a$ -particles, because the hardcore constraint leads to a change in the allowed momentum values when the total number of particles is changed.<sup>23</sup> To take the hardcore

nature of the bosons into account, we can postulate that the physical creation operator of the  $b$ -boson can be represented as

$$\psi_b^\dagger = b^\dagger a^\dagger = \bar{b}^\dagger e^{i(\sqrt{\pi}-\delta)\theta}. \quad (9)$$

With that definition,  $b$  is the “color-changing” operator for an existing sea particle, and in absence of any other interaction except the hardcore constraint the excitation of a  $b$ -particle would be equivalent to adding another sea boson and the only difference would be the additional energy cost  $\omega_0$ .

We are interested in the correlator  $\langle \psi_b^\dagger(x, t) \psi_b(0, 0) \rangle$  because it determines the “impurity” contribution to the longitudinal DSF

$$S^{zz}(\pi, \omega) \propto \int dx \int dt e^{i\omega t} \langle \psi_b^\dagger(x, t) \psi_b(0, 0) \rangle \quad (10)$$

Since the  $\bar{b}$  quasiparticles are free after the transformation, the correlator factorizes. One has  $\langle \bar{b}^\dagger(x, t) \bar{b}(0, 0) \rangle \propto \delta(x) e^{-i\omega_0 t}$ , where the Dirac delta-function  $\delta(x)$  is the consequence of irrelevance of the dispersion term in (5), so that

$$\langle \psi_b^\dagger(x, t) \psi_b(0, 0) \rangle \propto e^{-i\omega_0 t} \delta(x) / t^{\eta'}, \quad (11)$$

where

$$\eta' = \frac{1}{2K} \left(1 - \frac{KU_f}{\pi v_F}\right)^2 \quad (12)$$

is the “impurity exponent”. The longitudinal dynamical structure factor thus contains an edge singularity

$$S^{zz}(\pi, \omega) \propto \frac{1}{(\omega - \omega_0)^{\alpha'}} \quad \text{with} \quad \alpha' = 1 - \eta'. \quad (13)$$

The edge exponent  $\alpha'$ , in contrast to the low-energy edge exponent  $\alpha$ , depends not only on the TL liquid parameter  $K$ , but also on the Fermi velocity  $v_F$  and on the “host-impurity” interaction  $U_f$ . In the noninteracting hardcore case, which corresponds to  $U_f = 0$  and  $K = 1$ , this exponent takes the value  $\alpha' = \frac{1}{2}$ , in agreement with earlier studies.<sup>22,23,24</sup>

Comparing (13) and (4), one can see that the high-energy DSF exponent  $\alpha' = 1 - \eta'$  should be considerably smaller than the low-energy one  $\alpha = 2 - \eta$ . In our approach, this is a direct consequence of the dynamical localization of the “impurity”, which in turn followed from the non-relativistic form of the  $\mathcal{H}_b$  Hamiltonian (5). It is worthwhile to note that the same answer is obtained assuming that  $\mathcal{H}_b$  has a Lorentz-invariant form and describes massive field with mass  $\omega_0$  and characteristic limiting velocity  $c$ . In this latter case  $\langle \bar{b}^\dagger(x, t) \bar{b}(0, 0) \rangle \propto K_0(\omega_0 r/c)$ , where  $K_0$  is the Bessel function, and  $r = \sqrt{x^2 - c^2 t^2}$ , and one can show<sup>24</sup> that the corresponding Fourier transform yields the same asymptotic behavior (13).

### III. TECHNIQUE

We use the density matrix renormalization group (DMRG) method<sup>33,34</sup> to calculate the spectral function defined earlier. The DMRG works by truncating the Hilbert space of the system, based on selecting the optimal states from the Schmidt decomposition of the lattice as split into two (left and right) blocks. The method we use is a matrix product generalization of the “correction vector method”<sup>35</sup>, in which we calculate the Green’s function

$$G(q, \omega + i\delta) = \langle 0 | \hat{A}_q^\dagger \frac{1}{E_0 + \omega + i\delta - \hat{H}} \hat{A}_q | 0 \rangle \quad (14)$$

at a given frequency  $\omega$  with  $E_0$  being the ground state energy of the system and  $\delta$  a numerical broadening, via the so-called “correction vector”,

$$|c(w + i\delta)\rangle = (E_0 + w + i\delta - \hat{H})^{-1} \hat{A}_q |0\rangle, \quad (15)$$

which is determined by a standard linear solver (we used GMRES, but biconjugate gradient is also popular). In contrast to the traditional dynamical DMRG approach where the groundstate  $|0\rangle$ , Lanczos vector  $\hat{A}_q |0\rangle$  and correction vector are all determined simultaneously, the matrix product formulation allows the calculation to be split up, improving both the speed and accuracy (for a given size of the truncated Hilbert space) of the calculation. We first calculate the matrix product approximation to the groundstate  $|0\rangle$  by a standard DMRG calculation, so that we can apply  $\hat{A}_q$  exactly to give the Lanczos vector, which is independent of frequency. This is used as input to the correction vector solver which is trivially parallelizable over different frequencies, but we can also e.g., use a previously determined correction vector from a nearby frequency as the initial “guess” vector, additionally accelerating the calculation. The matrix product formulation provides good control over the errors, as the residual norm  $\| \hat{A}_q |0\rangle - (E_0 + w + i\delta - \hat{H}) |c(w + i\delta)\rangle \|$  can be calculated *exactly*. This is prohibitively difficult in the standard DMRG approach as it requires calculating the matrix elements of  $\hat{H}^2$  and the usual dynamical DMRG approximation  $\hat{H}^2 \simeq (P \hat{H} P^\dagger)^2$ , where  $P$  is the projector onto the truncated Hilbert space, is inadequate and produces an estimate for the residual norm that is many orders of magnitude too small. Details of this calculation will be provided elsewhere (see also reference [36] for a similar approach to this calculation). Given the correction vector, the Green’s function can be obtained via

$$G(q, \omega + i\delta) = \langle \hat{A}_q^\dagger | c(w + i\delta) \rangle, \quad (16)$$

from which the spectral function

$$S(q, \omega) = -\frac{1}{\pi} \lim_{\delta \rightarrow 0^+} \text{Im} G(q, \omega) \quad (17)$$

can be obtained.

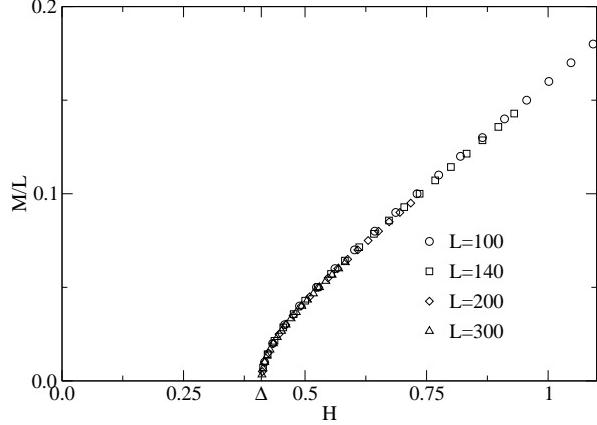


FIG. 1: Ground state magnetization per site versus magnetic field for different system sizes.

#### IV. RESULTS AND DISCUSSION

We start with the low-energy properties of the transversal DSF, which are better understood analytically, to show the validity of the method. First of all, we have to determine the total spin of the ground state depending on the applied field strength. In Fig. 1 we show the ground state magnetization  $M$  as a function of the magnetic field  $H$ ; the results for different system sizes are consistent, indicating that finite size effects in  $M(H)$  are small for  $L \gtrsim 100$ .

The exponent  $\eta$  can be obtained from the static transverse spin-spin correlation function  $\langle S^x(x)S^x(0) \rangle \sim |x|^{-\eta}$  which is easily accessible in DMRG calculations. From this the TLL parameter can be calculated via  $K = 1/(2\eta)$ . The values for  $\eta$  are shown in Fig. 2 we show our values for  $\eta$  and compare them with analytical results based on the effective description in the nonlinear sigma-model framework<sup>12</sup> as well as with the earlier DMRG results.<sup>13</sup> From this  $\eta$  we get a first estimate for the edge exponent  $\alpha$  via the second equation in Eq. (4).

A typical scan of the low energy-continuum of  $S^{+-}(k = \pi, \omega)$  is shown in Fig. 3 for a 200-site chain. The magnetic field applied is  $H = 0.54$  in units of the coupling constant leading to a ground state magnetization per site of  $M/L = 0.05$ .

The spectrum reveals a set of peaks at discrete frequency values, as one expects for a finite-size system. The peaks are nearly equidistant (in fact, the distance between the peaks decreases slightly with the frequency, which is naturally explained by the effective decrease of the Fermi velocity as the Fermi sea gets emptied by more and more particles being excited). From the energy difference of the first two peaks we extract the Fermi velocity  $v_F$ ; its dependence on the magnetic field is in good agreement with the results of Konik and Fendley<sup>12</sup> (see Fig. 4) if one sets their parameter  $v_0$  to 2.5. This parameter has the meaning of a bare spin velocity in the nonlinear sigma model description of Konik and Fendley,

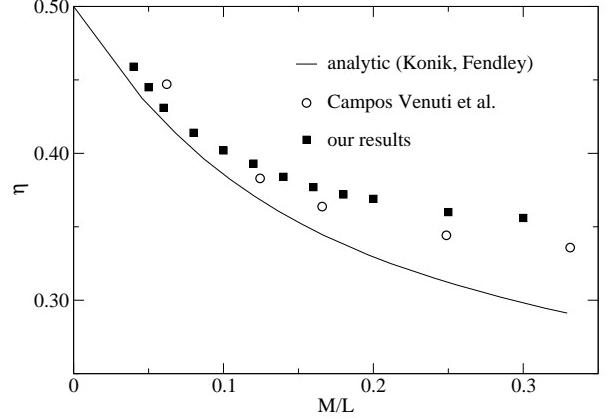


FIG. 2: Exponent  $\eta$  of the static correlation function. Solid line: results obtained from analytic calculations by Konik and Fendley<sup>12</sup> based on the effective nonlinear sigma-model description. Open circles: DMRG results for short chain lengths  $L < 80$  obtained by Campos Venuti *et al.*<sup>13</sup> Filled squares: our results obtained from DMRG calculations using chains of length  $L = 200$ .

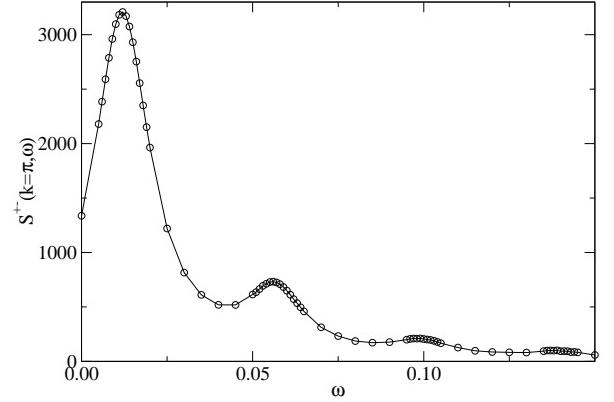


FIG. 3: Spectral function  $S^{+-}(k = \pi, \omega)$  for a 200-site chain at magnetic field  $H = 0.54$  leading to a ground state magnetization per site of  $M/L = 0.05$ . Here,  $\delta = 0.01$  and  $m = 300$  states were kept in the calculation.

and the value  $v_0 \approx 2.5$  agrees well with the known spin wave velocity  $v \approx 2.46$  of  $S = 1$  Haldane chain.<sup>37</sup>

One might be tempted to extract the edge exponent  $\alpha$  from the dependence of the peak heights in the spectral function (Fig. 3) on the frequency  $\omega$ . However, this is not a very good idea: although all these peaks are numerically broadened with the same constant  $\delta = 0.01$  for a  $L = 200$  site chain, they do not all show the same width as it would have been expected. With increasing frequency they get broader. This can be understood in the following way: The higher the excitation energy is, the more combinations exist to reach it by exciting several particle-hole pairs. In a system with an ideal linear dispersion the energies of all those combinations would be exactly the same and equal  $2\pi v_F n/L$  with  $n$  being

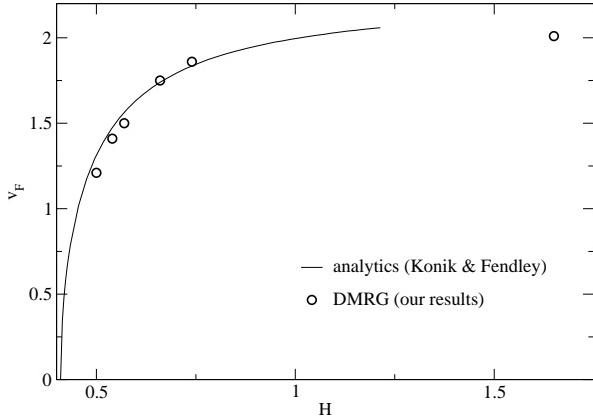


FIG. 4: Fermi velocity extracted from  $S^{+-}(k = \pi, \omega)$  as a function of magnetic field (open circles). The solid line corresponds to Eq.(40) of Konik and Fendley<sup>12</sup> with the bare spin wave velocity  $v_0 = 2.5$ .

some integer. In a real system the dispersion is not exactly linear, and those energies become slightly scattered around the  $2\pi v_F n/L$ , contributing an additional broadening to peaks with higher energy. Hence the height of the higher energy peaks is underestimated and thus the decay is overestimated leading to a value for the exponent  $\alpha$  being too large.

There is a much better way to determine the edge exponent, namely from the size dependence of the peak strength. The height of the first peak at  $\omega_1$  is given by

$$S^{+-}(k = \pi, \omega_1) \propto 1/\omega_1^\alpha.$$

With  $\omega_1 \propto v_F/L$  we find

$$S^{+-}(k = \pi, \omega_1) \propto L^\alpha$$

for fixed magnetization per site. This is shown in a log-log plot in Fig. 5. From calculations for different chain lengths  $L = 50, 100, 150, 200$  we find values for  $\alpha$  much closer to the expected value.

The values obtained from this  $L$ -fit and the expectations from  $\alpha = 2 - \eta$  are compared in Fig. 6. The agreement of both values is good for all  $M/L$  (deviation  $< 5\%$ ) and gets better for larger magnetizations. Having found a reliable way to extract  $\alpha$  we turn to the high-energy continuum in  $S^{zz}(k = \pi, \omega)$ .

Typical spectra for different magnetizations are shown in Fig. 7. The edge frequency shifts to higher energies with increasing magnetization. Due to the large energy the convergence of the algorithm is worse than for the previous continuum resulting in a significantly larger DMRG basis. Apart from the expected series of peaks these spectra show small additional peaks between each two peaks. These are finite-size artifacts that vanish for sufficiently large system sizes.

The Fermi velocity extracted from the upper continuum spectra is very similar to the one obtained from the low-energy continuum as shown in Fig. 8.

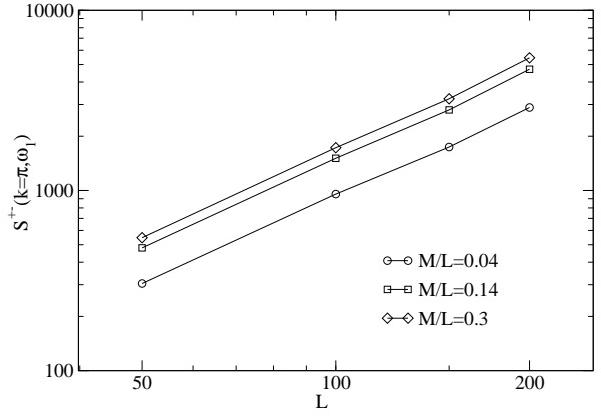


FIG. 5: Peak height of the first peak in  $S^{+-}(k = \pi, \omega)$  as function of the system size  $L$  for different magnetizations. Fitting this log-log plot by a straight line yields the edge exponent  $\alpha$ .

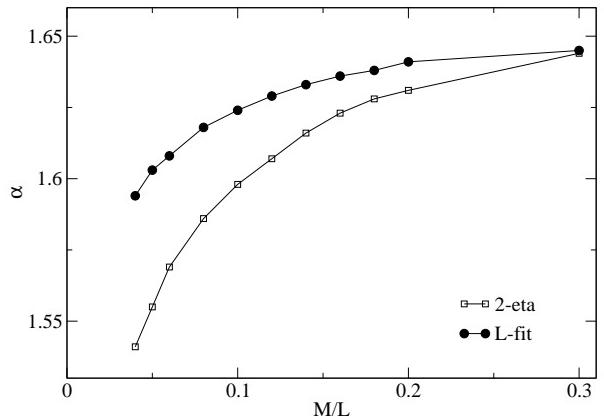


FIG. 6: Edge exponent  $\alpha$  obtained from fitting the height of the first peaks in the spectral function versus the chain length by a power law (full circles). The open squares were obtained using Eq.4.

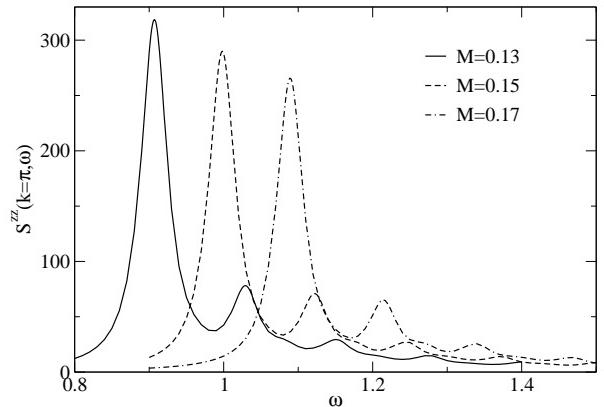


FIG. 7:  $S^{zz}(k = \pi, \omega)$  for different magnetizations. Here the numerical broadening is  $\delta = 0.02$  and  $m = 500$  states were kept in the reduced DMRG basis.

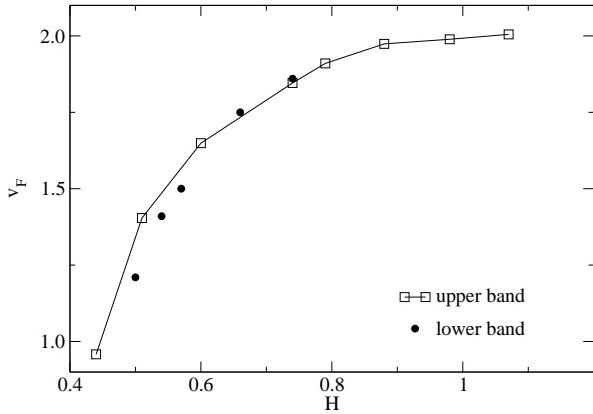


FIG. 8: Fermi velocities extracted from the low-energy spectrum (filled circles) and from the high energy one (open squares).

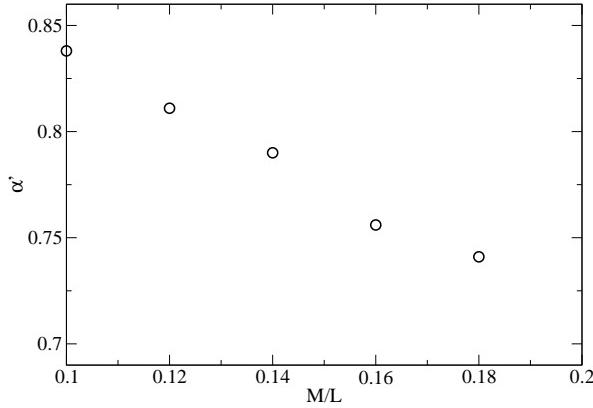


FIG. 9: The edge exponent of the high-energy continuum  $\alpha'$  obtained from the  $L$ -fit of the first peak height for different magnetizations.

Like in the low-energy continuum, the peaks get broader with increasing energy, making direct power-law fit of peak intensity vs frequency difficult. Thus, for determining the edge exponent  $\alpha'$  the same procedure based on the size dependence is used as in the previous case. From those fits we find the exponent as shown in Fig. 9.

As a further check for the consistency of our data, we show a fit of the high energy continuum for a magnetization per site  $M/L = 0.14$  calculated in a  $L = 100$  site chain. We have fitted the spectrum to a sum of Lorentzians with different widths and with a power-law decay of the peak intensity with the exponent fixed at the value  $\alpha' = 0.79$  obtained from the analysis of the size dependence of the peak heights. The peak widths and the true edge frequency  $\omega_0$  were used as fitting parameters. The result is shown in Fig. 11. Since the small shoulder at  $\omega \approx 1.13$  is a finite size effect it has not been fitted. The values obtained for the peak widths  $\gamma_i$  are  $\gamma_1 = 0.0207$ ,  $\gamma_2 = 0.0236$ ,  $\gamma_3 = 0.0442$ , and  $\gamma_4 = 0.0820$ . These widths

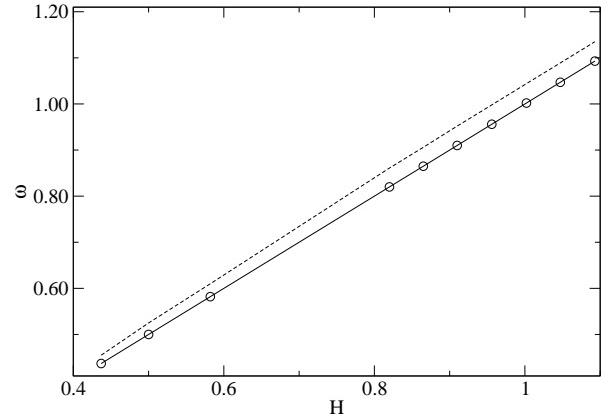


FIG. 10: Position of the first peak as function of the magnetic field (circles). The dashed line denotes  $\omega_0 = H$  as expected for the idealized hardcore boson model.<sup>22,23</sup>

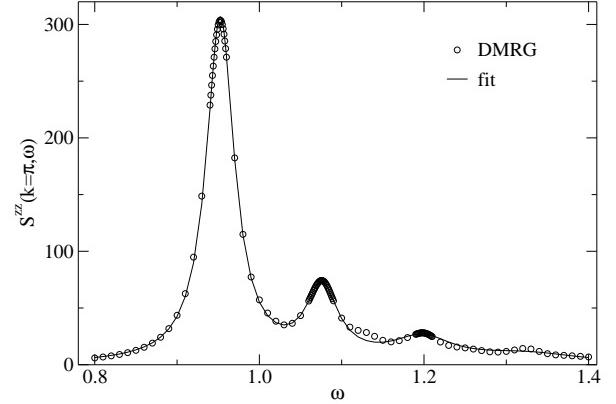


FIG. 11: Circles:  $S^{zz}(k = \pi, \omega)$  obtained with  $m = 500$  states in the DMRG basis. Solid line: Fit by a sum of Lorentzians. For fitting parameters see text.

and the independently obtained  $\alpha'$  provide an excellent fit. The true edge frequency  $\omega_0 = 0.929$  is slightly smaller than the position of the first peak  $\omega_1 = 0.952$ . To check the validity of this particular value we perform an  $L \rightarrow \infty$  extrapolation of  $\omega_1(L)$  which is supposed to yield the edge frequency. We find  $\omega_1(L \rightarrow \infty) = 0.935$  which is slightly larger than the one found from the fitting procedure.

Notably, the exponent  $\alpha'$  decreases with increasing magnetization unlike the edge exponent of the low-energy continuum. With the knowledge of the edge exponent  $\alpha'$ , the Fermi velocity  $v_F$  and the static exponent  $\eta$  we can extract the effective “host-impurity” interaction  $U_f$  using Eqs. (12), (13). The values of  $U_f$  extracted in that way lie between 7.7 and 8.3, which can be deemed approximately independent of the magnetization (within  $\pm 5\%$  accuracy).

The position of the first peak  $\omega_1$  (which serves as a crude approximation for the true edge frequency  $\omega_0$ ) as

a function of the magnetic field shows a clear linear dependence (see Fig. 10). It should be noted that a linear dependence  $\omega_0 = H$  has been obtained in the idealized hardcore bosonic model,<sup>22,23</sup> as well as in a bosonisation calculation<sup>24</sup> for a  $S = \frac{1}{2}$  ladder. The observed dependence is quite close to  $\omega_0 = H$  as seen in Fig. 10.

## V. SUMMARY

We have shown that the high-energy spectrum of a  $S = 1$  Heisenberg chain in a strong external magnetic field  $H$  exceeding the Haldane gap  $\Delta$  contains edge singularities, similar to those known to exist in the low-energy spectral response. It is found that in the frequency range  $\omega \gtrsim \Delta$  the longitudinal (with respect to the applied field) dynamical structure factor is dominated by the power-law singularity  $S^{\parallel}(q = \pi, \omega) \propto (\omega - \omega_0)^{-\alpha'}$ . It is shown that the edge exponent of the high-energy continuum  $\alpha'$  decreases with the magnetic field, consis-

tent with theoretical expectations. The edge frequency  $\omega_0$  is found to increase linearly with the magnetic field,  $\omega_0 \simeq cH$ , the coefficient  $c$  being close to 1, which agrees well with the predictions of Refs. 22,23,24. The existence of power-law continua with edge singularities at high energies should be a quite general feature, common for all one-dimensional gapped spin systems in high magnetic fields and directly related to the Tomonaga-Luttinger liquid character of the ground state at  $H > \Delta$ .

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